ABSTRACT

Method and system for processing and evaluating data from combination chromatographic and mass spectrometric data. The methods and system comprise data smoothing and determination of an quality factor for a chromatogram of a data set based on a determined entropy value. In one embodiment, the methods and system further comprise data baseline correction prior to entropy value determination. In a further embodiment, a correlation is determined between chromatograms processed according to the invention and one or more chromatograms of one or more data sets. Preferably, said correlation is performed using a multivariate analysis.

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